

**Gradient expansion of the Bloch propagator for position  
dependent effective mass hamiltonians in dimensions  $d = 1, 2, 3, 4$ .**

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**Abstract**

We derive the gradient expansion for the diagonal elements of the Bloch propagator up to order  $\hbar^2$ . We consider hamiltonians with position dependent effective mass and slowly varying local potential in spatial dimensions  $d = 1, 2, 3, 4$ . In our approach, we use the semiclassical  $\hbar$  expansion of the density matrix in [Phys. Rev. **A72**, 022508 2005] with the help of Laplace transform to derive such gradient expansion in the one-body potential and also in the effective mass distribution.

## I. INTRODUCTION

Quantum mechanical system with a spatially varying effective mass have attracted a lot of attention and inspired intense research activities during recent years. They are for instance very useful in the study of the physical properties of various microstructures and semiconductor interfaces in condensed matter. Special applications of these models are carried out in the study of electronic properties of semiconductors[1], quantum wells and quantum dots,[2],[19] 3He clusters,[3] quantum liquids,[4] graded alloys and semiconductor heterostructures,[5] ... etc. These applications stimulated a lot of work in the literature on the development of methods and techniques for studying systems with mass that depends on position. On the other hand, the Bloch propagator or its Fourier transform namely the Green function are of prime significance since they contain all quantum mechanical informations on the system. To our knowledge the existing list devoted to the study on the Bloch propagator of quantum systems involving position dependent effective mass is very short and is limited to the one dimensional case [10], [8]. This has motivated the present work to obtain approximate analytical expression for the propagator or at least for its diagonal parts in spatial dimension  $d$ . The resulting expression may constitute a good test for the exact results. To this end, we make use of a semiclassical approximation, to derive simple expressions for the diagonal elements of the Bloch propagator when the effective mass is allowed to be position dependent.

In a short, there exists a variety of procedures to generate the semiclassical  $\hbar$  expansion with a final objective being the  $\hbar$  expansion of the density matrix. We mention, for instance, the partition function method of Wigner-Kirkwood and further developed by Bhaduri and collaborators (see Ref.[11] and references cited therein), the Kirzhnits expansion using commutator formalism [see Ref. [12] and references cited therein] ,[9] ,[13] and the purely algebraic method introduced by Baraff and Borowich[14] and further developed by Grammaticos and Voros [15], based on the Wigner transform of operators. The latter method is particularly suitable for position dependent mass hamiltonians. These authors derived the semiclassical  $\hbar$  expansions for the 3-dimensional one particle density and also for other densities of physical interest when kinetic energy operator of one-particle hamiltonian comprises a spatially dependent effective mass. Later on, we have generalized[6] such expansion up to order  $\hbar^2$  for systems with effective mass distribution and reduced dimensionality, i.e,  $d = 1, 2$  dimensions. It should be noted that corrections of order  $\hbar^2$  generate not only second order gradient corrections in the one-body potential and also second order gradient corrections in the effective mass distribution. Here, we are interested in obtaining the gradient expansion of the diagonal elements for the Bloch propagator in  $d = 1, 2$  and 4 spatial dimensions for hamiltonians with position dependent mass (the result in  $d = 3$  is already known ).

The rest of the paper is organized as follows, In Section 2 we briefly recall some basic

definitions concerning the use of the Bloch propagator and its relationship to the density matrix. Starting from the semiclassical  $\hbar$  expansion for the particle density, we derive in Section 3 the corresponding expansion up to second order in  $\hbar$  for the diagonal elements of the Bloch propagator in  $d = 1, 2$  and 4 spatial dimensions for hamiltonians with position dependent mass. A general analytical expression is found for the latter quantity in terms of the dimension  $d$  of the considered space. Section 4 provides an illustrative numerical example. Finally, a conclusion is given in Section 5.

## II. BASIC CONCEPTS

Consider a system of  $N$  noninteracting fermions with spatially varying effective mass  $m^*(\vec{r})$  moving in a smooth potential  $U(\vec{r})$ . Throughout the present study, we shall be working with the one-body Hamiltonian given by

$$H = -\frac{\hbar^2}{2m_0} \vec{\nabla} \cdot f(\vec{r}) \vec{\nabla} + U(\vec{r}) \quad (1)$$

where  $f(\vec{r}) = m_0/m^*(\vec{r})$  denotes the ratio of the free particle mass  $m_0$  to the position dependent effective mass  $m^*(\vec{r})$  and where we use, as done in the majority of work on the subject, the symmetric ordering form of mass and momentum in the kinetic energy term of  $H$ .

Let  $\varphi_n(\vec{r})$  be the eigenfunctions of  $H$  and  $\varepsilon_n$  the corresponding eigenvalues, i.e;  $H\varphi_n(\vec{r}) = \varepsilon_n\varphi_n(\vec{r})$ , at zero temperature the single-particle density matrix of the system  $\rho(\vec{r}, \vec{r}')$ , is given by

$$\rho(\vec{r}, \vec{r}') = \sum_n \varphi_n^*(\vec{r}) \varphi_n(\vec{r}') \Theta(\lambda - \varepsilon_n) \quad (2)$$

where  $\lambda$  is the Fermi energy and  $\Theta(x)$  is the Heaviside step function which allows to restrict the sum over occupied states only.

Given the above density matrix, the Bloch propagator  $C(\vec{r}, \vec{r}'; \beta)$ , defined as [see for instance [11]]

$$C(\vec{r}, \vec{r}'; \beta) := \langle \vec{r} | \exp(-\beta H) | \vec{r}' \rangle = \sum_n \varphi_n^*(\vec{r}) \varphi_n(\vec{r}') \exp(-\beta \varepsilon_n) \quad (3)$$

can be obtained through the Laplace transform result

$$C(\vec{r}, \vec{r}'; \beta) = \beta \int_0^\infty d\lambda e^{-\beta\lambda} \rho(\vec{r}, \vec{r}') \quad (4)$$

It should be noted that, in quantum statistics and thermodynamics,  $\beta$  is an inverse of temperature:  $\beta = 1/k_B T$  with  $k_B$  is the Boltzmann constant but if we now replace  $\beta$  in equation (3) by  $\beta \rightarrow it/\hbar$ , the resulting propagator  $K(\vec{r}, \vec{r}'; t)$  describes the propagation

of the single particle from  $\vec{r}' \rightarrow \vec{r}$  in time  $t$ . However in the subsequent analysis  $\beta$  is to be viewed as a complex parameter. The interest in the Bloch propagator is that it contains all quantum mechanical informations[21],[11],[22], from which the density matrix  $\rho(\vec{r}, \vec{r}')$  in Eq. (2) may be obtained by suitable inverse Laplace transform, that is

$$\rho(\vec{r}, \vec{r}') = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\beta\lambda} \frac{C(\vec{r}, \vec{r}', \beta)}{\beta} d\beta, \quad c > 0 \quad (5)$$

where, to carry out the complex integration in equation (5), the parameter  $\beta$ , as stated before, is considered as a mathematical variable which is taken to be complex.

Putting  $\vec{r}' = \vec{r}$  in equation (4), we evidently get

$$C(\vec{r}; \beta) = \beta \int_0^\infty d\lambda e^{-\beta\lambda} \rho(\vec{r}) \quad (6)$$

where henceforth  $C(\vec{r}; \beta)$  denotes the diagonal elements of the Bloch propagator, called also the Slater sum, and  $\rho(\vec{r})$  being the local particle density.

In the above spirit, all the results are formally exact, we shall in the next section use them within the framework of gradient expansion. Notice that, for the case of constant effective mass hamiltonians the local version of equation (5) has been used to calculate the density from the Bloch propagator[20]. In the present context dealing with position dependent hamiltonians, we invert the procedure and we shall use equation (6) to get the Bloch propagator since, as stated before, the gradient expansions of the local density are known.

### III. GRADIENT EXPANSION FOR THE DIAGONAL ELEMENTS OF THE BLOCH PROPAGATOR FOR SPATIALLY VARYING EFFECTIVE MASS HAMILTONIANS IN DIMENSIONS D=1,2,3,4.

In this section explicit  $\hbar$  expansions will be presented for the diagonal elements of the Bloch propagator through the use of equation (6). For that, we directly use the  $\hbar$  expansions of the particle density  $\rho(\vec{r})$  derived in[6]. In one spatial dimension it is given up to order  $\hbar^2$  by [see equation (A5) of reference [6]]

$$\begin{aligned}
\rho_{d=1}(x) = & \frac{1}{\pi} \sqrt{\frac{2m_0}{\hbar^2 f}} (\lambda - V)^{+1/2} \theta(\lambda - V) + \\
& \sqrt{\frac{\hbar^2 f}{2m_0}} \left\{ \left[ \frac{1}{32\pi} \frac{1}{f^2} \left( \frac{df}{dx} \right)^2 (\lambda - V)^{-1/2} + \frac{1}{48\pi} \left( 2 \frac{d^2 V}{dx^2} + \frac{1}{f} \frac{df}{dx} \frac{dV}{dx} \right) (\lambda - V)^{-3/2} + \right. \right. \\
& \left. \left. \frac{1}{32\pi} \left( \frac{dV}{dx} \right)^2 (\lambda - V)^{-5/2} \right] \theta(\lambda - V) - \right. \\
& \left. \left[ \frac{1}{24\pi} \left( 2 \frac{d^2 V}{dx^2} + \frac{1}{f} \frac{df}{dx} \frac{dV}{dx} \right) (\lambda - V)^{-1/2} + \frac{1}{24\pi} \left( \frac{dV}{dx} \right)^2 (\lambda - V)^{-3/2} \right] \delta(\lambda - V) + \right. \\
& \left. \frac{1}{24\pi} \left( \frac{dV}{dx} \right)^2 (\lambda - V)^{-1/2} \frac{\partial \delta(\lambda - V)}{\partial \lambda} \right\} \quad (7)
\end{aligned}$$

Here the potential  $V(\vec{r})$  is related to the one-body potential  $U(\vec{r})$  in Eq. (1) by  $V(\vec{r}) = U(\vec{r}) + \frac{\hbar^2}{8m_0} \vec{\nabla}^2 f(\vec{r})$  [6] and  $\delta$  is the Dirac distribution. Notice that, here we do not include the spin degeneracy (factor of two for spin half particles) in the expression of the particle density in (7) as was done in [6]. Next, It is easy to verify that, the equation may be simplified to

$$\begin{aligned}
\rho_{d=1}(x) = & \frac{1}{\pi} \sqrt{\frac{2m_0}{\hbar^2 f}} (\lambda - V)^{+1/2} \theta(\lambda - V) + \\
& \sqrt{\frac{\hbar^2 f}{2m_0}} \left\{ \frac{1}{16\pi} \frac{1}{f^2} \left( \frac{df}{dx} \right)^2 \left[ \frac{\partial (\lambda - V)^{+1/2} \theta(\lambda - V)}{\partial \lambda} \right] - \right. \\
& \frac{1}{24\pi} \left( 2 \frac{d^2 V}{dx^2} + \frac{1}{f} \frac{df}{dx} \frac{dV}{dx} \right) \left[ \frac{\partial (\lambda - V)^{-1/2} \theta(\lambda - V)}{\partial \lambda} \right] + \\
& \left. \frac{1}{24\pi} \left( \frac{dV}{dx} \right)^2 \left[ \frac{\partial^2 (\lambda - V)^{-1/2} \theta(\lambda - V)}{\partial \lambda^2} \right] \right\} \quad (8)
\end{aligned}$$

which can be alternatively rewritten as

$$\begin{aligned}
\rho_{d=1}(x) = & \frac{1}{\pi} \sqrt{\frac{2m_0}{\hbar^2 f}} (\lambda - V)^{1/2} \theta(\lambda - V) + \\
& \sqrt{\frac{\hbar^2 f}{2m_0}} \left\{ \frac{1}{16\pi} \frac{1}{f^2} \left( \frac{df}{dx} \right)^2 \left[ \frac{\partial (\lambda - V)^{+1/2} \theta(\lambda - V)}{\partial \lambda} \right] - \right. \\
& \frac{1}{12\pi} \left( 2 \frac{d^2 V}{dx^2} + \frac{1}{f} \frac{df}{dx} \frac{dV}{dx} \right) \left[ \frac{\partial^2 (\lambda - V)^{+1/2} \theta(\lambda - V)}{\partial \lambda^2} \right] + \\
& \left. \frac{1}{12\pi} \left( \frac{dV}{dx} \right)^2 \left[ \frac{\partial^3 (\lambda - V)^{+1/2} \theta(\lambda - V)}{\partial \lambda^3} \right] \right\} \quad (9)
\end{aligned}$$

The reason that we have displayed the result in the form (9) is that, for the case of a constant effective mass our expression of the density reduces exactly to the one given by equation (12) of [9] in one spatial dimension, where the latter density was obtained through a different semiclassical method namely the Kirzhnits expansion.

To obtain the local Bloch density, we use for the density the form in (8) rather than (9) and substitute it into Eq. (6) and then we use the following property of Laplace transforms [11], [17] applied to each term of the expansion

$$\int_0^\infty d\lambda e^{-\beta\lambda} [(\lambda - V(\vec{r}))^\nu \theta(\lambda - V(\vec{r}))] = \frac{\Gamma(\nu + 1)}{\beta^{\nu+1}} e^{-\beta V(\vec{r})} \quad (10)$$

and using obvious notations, we then obtain

$$C_{d=1}(\vec{r}; \beta) = \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{1/2} e^{-\beta V(\vec{r})} \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \frac{3}{4} \left( \frac{1}{f} \frac{df}{dx} \right)^2 \beta + \left[ \left( -\frac{1}{f} \frac{df}{dx} \cdot \frac{dV}{dx} \right) - 2 \left( \frac{d^2 V}{dx^2} \right) \right] \beta^2 + \left( \frac{dV}{dx} \right)^2 \beta^3 \right\} \right] \quad (11)$$

Let us now come to the two dimensional case and we write down the corresponding  $\hbar$  expansions of the local density given by Eq. (28) of [6]

$$\begin{aligned} \rho_{d=2}(\vec{r}) &= \frac{m_0}{2\pi\hbar^2 f} (\lambda - V) \Theta(\lambda - V) + \frac{1}{48\pi} \left[ \left( \frac{\vec{\nabla} f}{f} \right)^2 - \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \Theta(\lambda - V) \\ &\quad - \frac{1}{24\pi} (\vec{\nabla}^2 V) \delta(\lambda - V) + \frac{1}{48\pi} (\vec{\nabla} V)^2 \frac{\partial \delta(\lambda - V)}{\partial \lambda} \end{aligned} \quad (12)$$

Plugging Eq.(12) into (6) with the use of Laplace transform identity (10), we find for the local Bloch propagator

$$C_{d=2}(\vec{r}; \beta) = \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right) e^{-\beta V(\vec{r})} \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \left[ \left( \frac{\vec{\nabla} f}{f} \right)^2 - \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta - 2 (\vec{\nabla}^2 V) \beta^2 + (\vec{\nabla} V)^2 \beta^3 \right\} \right] \quad (13)$$

For the  $d = 3$  case, the expression of the local density up to order  $\hbar^2$  [see for instance [16] and references cited therein]

$$\begin{aligned} \rho_{d=3}(\vec{r}) &= \frac{1}{6\pi^2 \hbar^3} \left( \frac{2m_0}{f} \right)^{3/2} (\lambda - V)^{3/2} \Theta(\lambda - V) + \\ &\quad \frac{1}{24\pi^2 \hbar} \sqrt{\frac{m_0}{2f}} \left\{ \left[ \frac{7}{4} \left( \frac{\vec{\nabla} f}{f} \right)^2 - 2 \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] (\lambda - V)^{1/2} \Theta(\lambda - V) + \right. \\ &\quad \left. \left[ \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2(\vec{\nabla}^2 V) \right] (\lambda - V)^{-1/2} \Theta(\lambda - V) - \frac{1}{4} (\vec{\nabla} V)^2 (\lambda - V)^{-3/2} \Theta(\lambda - V) \right\} \end{aligned} \quad (14)$$

Substituting Eq. (14) into (6) followed by the use of (10), we get

$$C_{d=3}(\vec{r}; \beta) = \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{3/2} e^{-\beta V(\vec{r})} \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \left[ \frac{7}{4} \left( \frac{\vec{\nabla} f}{f} \right)^2 - 2 \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta + \left[ \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left( \vec{\nabla}^2 V \right) \right] \beta^2 + (\vec{\nabla} V)^2 \beta^3 \right\} \right] \quad (15)$$

It is interesting to observe that the results given respectively in equations (11), (13) and (15) can be written down in terms of the dimensionality  $d$  of the space as follows

$$C_d(\vec{r}; \beta) = \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{d/2} e^{-\beta V(\vec{r})} \times \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \left[ \frac{(d-1)^2 + 3}{4} \left( \frac{\vec{\nabla} f}{f} \right)^2 + (1-d) \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta + \left[ (d-2) \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left( \vec{\nabla}^2 V \right) \right] \beta^2 + (\vec{\nabla} V)^2 \beta^3 \right\} \right] \quad (16)$$

We have looked whether the above equation is valid for higher dimensions or at least for  $d = 4$ . For that, we have make use of the semiclassical approach in Ref. [15] to write down the local density up to order  $\hbar^2$  in  $d = 4$  dimension. We have obtained

$$\rho_{d=4}(\vec{r}) = \frac{m_0^2}{8\pi^2 \hbar^4 f^2} (\lambda - V)^2 \theta(\lambda - V) + \frac{m_0}{32\pi^2 \hbar^2 f} \left[ \left( \frac{\vec{\nabla} f}{f} \right)^2 - \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] (\lambda - V) \theta(\lambda - V) + \frac{m_0}{48\pi^2 \hbar^2 f} \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) \theta(\lambda - V) - \frac{m_0}{48\pi^2 \hbar^2 f} \left( \vec{\nabla}^2 V \right) \theta(\lambda - V) + \frac{m_0}{96\pi^2 \hbar^2 f} \left( \vec{\nabla} V \right)^2 \delta(\lambda - V) \quad (17)$$

Here  $\vec{\nabla}$  stands for the gradient in four dimensions. Having the density, we follow the same derivations as done for  $d = 1, 2, 3$  to obtain the corresponding local Bloch propagator, it yields

$$C_{d=4}(\vec{r}; \beta) = \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^2 e^{-\beta V(\vec{r})} \times \left[ 1 + \frac{\hbar^2}{24m_0} \left\{ 3 \left[ \left( \frac{\vec{\nabla} f}{f} \right)^2 - \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta + \left[ 2 \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left( \vec{\nabla}^2 V \right) \right] \beta^2 + (\vec{\nabla} V)^2 \beta^3 \right\} \right] \quad (18)$$

It is easy to check that, setting  $d = 4$  in Eq.(16), one recovers the result in (18). Hence our expression given in (16) holds true for  $d = 1, 2, 3, 4$ . Notice that, in equation (16) unlike the position dependent mass terms, the remaining terms involving gradients of the potential do not depend on the dimension  $d$  of the considered space.

The interested reader may have noticed that the local Bloch density in Eq. (16) is expressed in terms of  $V(\vec{r}) = U(\vec{r}) + \frac{\hbar^2}{8m_0} \vec{\nabla}^2 f(\vec{r})$  and for practical use it is interesting to re-express it in terms of the original one body potential  $U(\vec{r})$ . Upon substitution, equation (16) becomes then

$$\begin{aligned}
C_d(\vec{r}; \beta) &= \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{d/2} e^{-\beta U(\vec{r})} \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \left[ \frac{(d-1)^2 + 3}{4} \left( \frac{\vec{\nabla} f}{f} \right)^2 + (1-d) \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta + \right. \right. \\
&\quad \left. \left[ (d-2) \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left( \vec{\nabla}^2 V \right) \right] \beta^2 + (\vec{\nabla} V)^2 \beta^3 \right\} \right] e^{-\beta \frac{\hbar^2}{8m_0} \vec{\nabla}^2 f(\vec{r})} \\
&= \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{d/2} e^{-\beta U(\vec{r})} \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \left[ \frac{(d-1)^2 + 3}{4} \left( \frac{\vec{\nabla} f}{f} \right)^2 + (1-d) \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta + \right. \right. \\
&\quad \left. \left[ (d-2) \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left( \vec{\nabla}^2 V \right) \right] \beta^2 + (\vec{\nabla} V)^2 \beta^3 \right\} \right] \left( 1 - \beta \frac{\hbar^2}{8m_0} \vec{\nabla}^2 f \right) \quad (19)
\end{aligned}$$

where in getting the second form, use has been made of the Taylor expansion up to order  $\hbar^2$  of  $\exp(-\beta \frac{\hbar^2}{8m_0} \vec{\nabla}^2 f) \approx 1 - \beta \frac{\hbar^2}{8m_0} \vec{\nabla}^2 f$ . Since, the terms involving  $\vec{\nabla} V$  and  $\vec{\nabla}^2 V$  are of order  $\hbar^2$ , we need only replace them in Eq. (19) by their leading terms, i.e;  $\vec{\nabla} V = \vec{\nabla} U + O(\hbar^2)$  and  $\vec{\nabla}^2 V = \vec{\nabla}^2 U + O(\hbar^2)$ . This leads finally, after simple rearrangements, up to order  $\hbar^2$

$$\begin{aligned}
C_d(\vec{r}; \beta) &= \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{d/2} e^{-\beta U} \left[ 1 + \frac{\hbar^2 f}{24m_0} \left\{ \left[ \frac{(d-1)^2 + 3}{4} \left( \frac{\vec{\nabla} f}{f} \right)^2 - (d+2) \left( \frac{\vec{\nabla}^2 f}{f} \right) \right] \beta + \right. \right. \\
&\quad \left. \left[ (d-2) \left( \frac{\vec{\nabla} f \cdot \vec{\nabla} U}{f} \right) - 2 \left( \vec{\nabla}^2 U \right) \right] \beta^2 + (\vec{\nabla} U)^2 \beta^3 \right\} \right] \quad (20)
\end{aligned}$$

where we recall that  $f(\vec{r}) = m_0/m^*(\vec{r})$ . As can be seen the above local Bloch density receives explicit contributions from the spatially varying effective mass  $m^*(\vec{r})$  not only at zero order, through the term proportional to  $f^{-d/2}$  and also from terms of order  $\hbar^2$  proportional to  $\vec{\nabla} f$  and  $\vec{\nabla}^2 f$ . The above equation is the main result of the present study. For  $d = 3$ , our expression reduces to the one obtained long time ago in the context of nuclear physics[23].

#### IV. NUMERICAL EXAMPLE

In this section, we want to test numerically the importance of the position dependent effective mass terms in the resultant propagator (20). For that, we need as an input a given effective mass  $m^*$  and potential  $U$ . As an illustration we focus on one-dimensional systems with mass distribution  $m^*(x)$  and we choose  $U(x)$  so that equation (1) possesses exact analytical solution. In Ref. [24], Alhaidari solved exactly equation



(1), for a large class of potentials, by means of an elegant method called point canonical transformations (PCT). Let us briefly sketch this technique. Under the following (PCT),  $y = \int (f(x))^{-\frac{1}{2}} dx$  and  $\varphi_n(x) = (f(x))^{-\frac{1}{4}} \psi_n(y)$ , the Schrödinger equation (1) with spatially mass distribution  $m^*(x) = m_0/f(x)$  and potential  $U(x)$ , is mapped to a Schrödinger equation with a constant mass  $m_0$ , so that,  $\left[-\frac{\hbar^2}{2m_0} \frac{d^2}{dy^2} + \tilde{U}(y)\right] \Psi_n(y) = E_n \Psi_n(y)$ , with  $U(x) = \tilde{U}(y) + \frac{\hbar^2}{8m(x)} \left[ \frac{1}{m(x)} \frac{d^2 m(x)}{dx^2} - \frac{7}{4m^2(x)} \left( \frac{dm(x)}{dx} \right)^2 \right]$  and  $E_n = \epsilon_n$ . Taking for the constant mass problem the harmonic oscillator potential  $\tilde{U}(y) = m_0 \omega^2 y^2 / 2$ , Alhaidari obtained the solutions for the Oscillator class for a given  $m^*(x)$ . Let us now take the specific mass distribution used in [24].

$$m(x) = m_0 \left( \frac{\gamma + x^2}{1 + x^2} \right)^2 \quad m(\pm\infty) = m_0 \quad (27)$$

from which we get  $f(x) = ((1 + x^2)/(\gamma + x^2))^2$  with  $\gamma$  being a real constant parameter, one then obtains  $y = x + (\gamma - 1) \arctan(x)$ . Note that when  $\gamma = 1.0$  equation (27) gives a constant effective mass  $m(x) = m_0$ . In terms of  $f(x)$  and its derivatives, the above potential  $U(x)$  reads then

$$U(x) = \frac{m_0 \omega^2}{2} [x + (\gamma - 1) \arctan(x)]^2 + \frac{\hbar^2}{8m_0} \left[ -\frac{d^2 f(x)}{dx^2} + \frac{1}{f(x)} \left( \frac{df(x)}{dx} \right)^2 \right] \quad (28)$$

In Figure 1., we plot the ratio  $f(x) = m_0/m(x)$  from Eq.(27) as a function of the spatial coordinate  $x$  for values of  $\gamma = 0.6, 0.8, 1.0$ . Setting the parameters  $\omega$  and  $\beta$  to 1, we plot in Figure 2. the Bloch density  $C_{d=1}(x; \beta)$  of Eq. (20) as a function of  $x$  for values of  $\gamma = 0.6, 0.8, 1.0$ . Here we consider particle of unit free mass  $m_0 = 1$ , and the Planck constant is set to 1. As is shown in this figure the presence of spatially varying effective mass may lead to important deviations locally with respect to the constant mass case. We also display in Figure 3. the second order  $\hbar^2$  term of the Bloch density, which using Eq. (20) is given by  $\delta C_{d=1}(x; \beta) = \frac{\hbar^2 f}{24m_0} \left( \frac{m_0}{2\pi\hbar^2 f \beta} \right)^{1/2} e^{-\beta U} \left\{ \left[ \frac{3}{4} \left( \frac{1}{f} \frac{df}{dx} \right)^2 - \frac{3}{f} \frac{d^2 f}{dx^2} \right] \beta + \left[ \left( -\frac{1}{f} \frac{df}{dx} \cdot \frac{dU}{dx} \right) - 2 \left( \frac{d^2 U}{dx^2} \right) \right] \beta^2 + \left( \frac{dU}{dx} \right)^2 \beta^3 \right\}$ . Deviations from the constant effective mass case are clearly exhibited at this order.

## V. CONCLUSION

In the present study we have derived the gradient expansion up to order  $\hbar^2$ , for the diagonal elements of the Bloch propagator for hamiltonians with position dependent mass. Our main result is summarized by equation (20) valid for spatial dimensions  $d = 1, 2, 3, 4$ . This result is valid for arbitrary one-body potential  $U(\vec{r})$  and spatially varying effective mass  $m^*(\vec{r})$ .

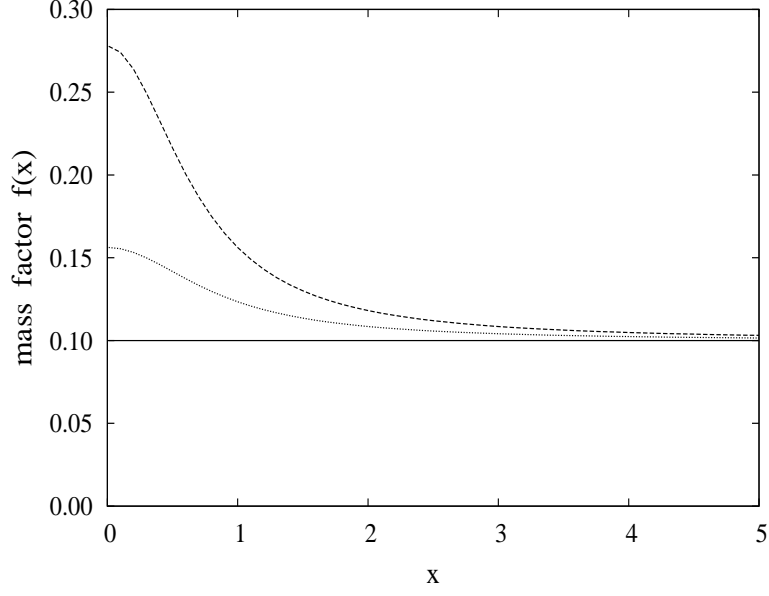


FIG. 1: A plot of position dependent effective mass ratio  $f(x) = m_0/m^*(x) = ((1+x^2)/(\gamma+x^2))^2$ . The solid curve is at value  $\gamma = 1$ , the dot curve is at value  $\gamma = 0.8$  and the dash curve is at value  $\gamma = 0.6$

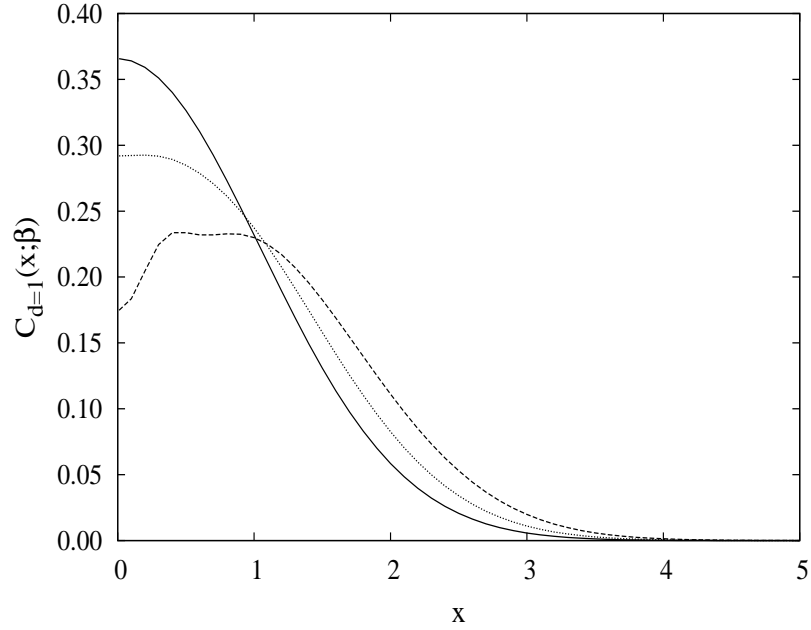


FIG. 2: A Plot of The local Bloch density  $C_{d=1}(x; \beta)$  with  $\omega = 1$ ,  $\beta = 1$ . Solid line correspond to  $\gamma = 1$ , dotted line  $\gamma = 0.8$  and dashed line  $\gamma = 0.6$ .

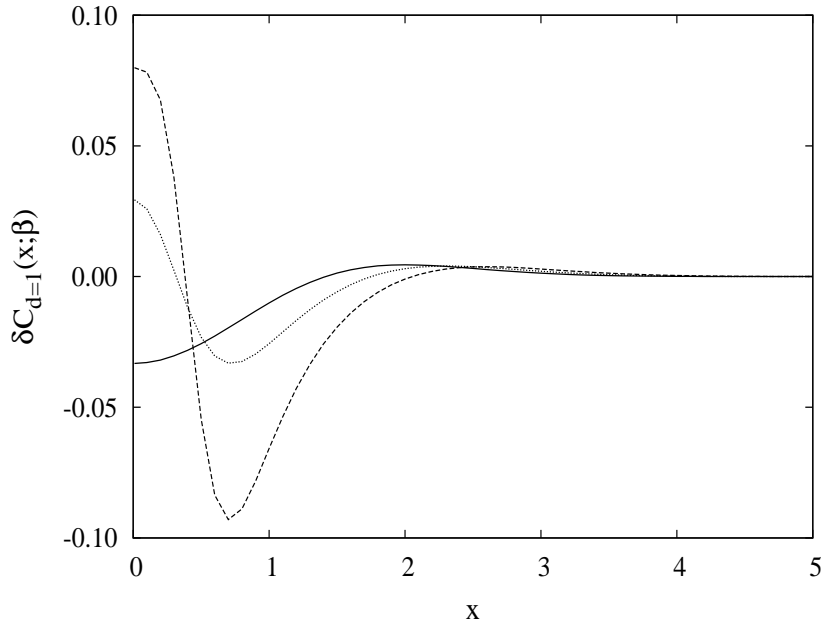


FIG. 3: The second order contribution to the Bloch density in figure 2  $\delta C_{d=1}(x; \beta)$  for values of  $\gamma = 0.6, 0.8, 1.0$  corresponding respectively to dashed, dotted and solid lines.

We have explicitly shown that, for  $d = 1$  and constant effective mass the expressions of the semiclassical densities derived respectively within the algebraic method due to Baraff and Borowich[14] and the Kirzhnits expansion are identical up to order  $\hbar^2$ . This would be certainly true for higher dimensions.

The results we have obtained would constitute useful approximation to the exact calculation of propagator or Green functions [10],[8] for hamiltonians with spatially varying mass.

An interesting extension of the present study will be the derivation of the semiclassical expansion for the non-diagonal elements  $C(\vec{r}, \vec{r}'; \beta)$  of the Bloch propagator.

## VI. REFERENCES

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- [1] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructure (Les Editions de Physique, Les Ulis, France, 1988)

- [2] L. Serra and E. Lipparini, *Europhys. Lett.* **40**, 667 (1997); P. Harrison, *Quantum Wells, Wires and Dots* (John Wiley and Sons, 2000)
- [3] M. Barranco, M. Pi, S. M. Gatica, E. S. Hernandez, and J. Navarro, *Phys. Rev. B* **56**, 8997 (1997), T. Gora, and F. Williams, *Phys. Rev.* **177**, 11979 (1969)
- [4] F. Arias de Saavedra, J. Boronat, A. Polls, and A. Fabrocini, *Phys. Rev. B* **50**, 4248 (1994)
- [5] C. Weisbuch and B. Vinter, *Quantum Semiconductor Heterostructures* (Academic Press, New York, 1993)
- [6] K. Berkane and K. Bencheikh, *Phy. Rev. A* **72**, 022508 2005
- [7] K. Bencheikh, K. Berkane, and S. Bouizane, *J. Phys. A* **37**, 10719 2004 .
- [8] N. Bouchemla and L. Chetouani, *Acta Physica Polonica B* **40** 2711 (2009)
- [9] L. Salasnich, *J. Phys. A: Math. and Theor* **40**, 9987 (2007).
- [10] A.D. Alhaidari, *Int. J. Theor. Phys.* **42** 2999 (2003)
- [11] M. Brack, R.K. Bhaduri, *Semiclassical Physics, Frontiers in Physics*, vol. 96, Westview, Boulder 2003
- [12] R.M. Dreizler and E.K.U. Gross, *Density Functional Theory* ( Springer-Verlag, Berlin 1990
- [13] A. Putaja, E. Räsänen, R. van Leeuwen, J. G. Villhena, and M. A. L. Marques, *Phys. Rev. B* **85**, 165101 (2012)
- [14] G. Baraff and S. Borowich, *Phys. Rev.* **121** 1704 (1961)
- [15] B. Grammaticos and A. Voros, *Ann. Phys.* **123** (1979) 359
- [16] K. Bencheikh, J. Bartel and P. Quentin, *Nucl. Phys A* **764** (2006) 79
- [17] M. Abramowitz and I. A. Stegun: *Handbook of Mathematical Functions* (Dover Publications, 9th printing, New York, 1970).
- [18] Gradshteyn I S and Ryzhik I M 1994 *Table of Integrals, Series, and Products* (Academic Press, New York, 5th edition).
- [19] R. Khordad, *Eur. Phys. J. B* **85** (2012)114; R. Khordad, *Physica B* **406** (2011) 3911–3916
- [20] A. Holas and N. H. March, *Philosophical Magazine B* **69** (1994) 787-798
- [21] N H March and W H Young, *Nucl. Phys.* **12** 237 (1959)
- [22] P. Shea and B. van Zyl, *J. Phys. A: Math. Theor.* **40** 10589 (2007); P. Shea and B. van Zyl, *J. Phys. A: Math. Theor.* **41** 135305 (2008).
- [23] M. Brack, B.K. Jennings and Y.H. Chu, *Phys. Lett.* **65B** (1976) 1.
- [24] A D. Alhaidari, *Phys. Rev. A* **66**, 042116 (2002)